Supporting Information

For

Congener-specific Mother-Fetus Distribution, Placental Retention, and Transport of C_{10-13} and C_{14-17} Chlorinated Paraffins in Pregnant Women

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Method

The quantification and analytical separation of chlorinated paraffins (CPs) in environmental and biological samples are extremely difficult because CPs are the most complex industrial mixtures which contain thousands of congeners and isomers. Currently, advance instruments (i.e. GCxGC-ECNI-HRTOF-MS, APCI-Orbitrap-MS, APCI-qTOF-MS, and LC-ESI-Orbitrap-MS, etc.) with high-resolution mass spectrometry are used for effective and selective analysis to accurately detect CPs, but these instruments are not available in many laboratories due to the high costs. The electron capture negative ionization with low-resolution mass spectrometry (ECNI-LRMS) is well-suited for routine analysis and widely used for accurate detection of CPs[1], but this method increases the risk of interference from other polychlorinated compounds and CPs. In this study, the analytical method combined with a mathematical calculation reported by Reth and Oehme [2,3] and Zeng et al., [4] was used to eliminate the overlapping interferences.

Instrumental Analysis and Quantification.

A 1 µL aliquot of the sample volume was injected into an HP-5MS UI (30 m, 0.25 mm, 0.25 µm) capillary column in the splitless mode. The injector temperature was set to 275 °C, and the carrier gas (Helium) flow rate was kept constant at 1.0 mL min^{-1}. The initial oven temperature was programed to 100°C for 1 min and then increased at a rate of 30°C/min^{-1} to 160°C (held for 5 min). Then the temperature was ramped up to 310°C at a rate of 30°C/min (held for 17 min). The source parameters were: ion source temperature 250°C; ionization energy 149.7 eV; ionization current 49.4 µA, and quadrupole temperature150°C. The two most abundant isotopes of the

$[M\text{-}Cl]^-$ ions of the SCCP and MCCP congener groups with 5-10 chlorine atoms were monitored in the selected ion monitoring (SIM) mode, the highest and second most abundant isotope ions of $[M\text{-}Cl]^-$ were used for quantification and confirmation, respectively (Table S3). [5,6] SCCPs and MCCPs contain thousands of homologues, complicating the congener-specific analysis of the complex mixture of CPs. The simultaneous analysis of SCCP congeners can interfere with MCCP congeners with similar mass and different molecular formula when LRMS in ECNI mode was employed. The interferences between SCCP and MCCP congener groups from the same nominal mass with five carbon atoms more and two chlorine atoms less could occur, which decreases the instrument sensitivity when simultaneously detecting SCCPs and MCCPs, due to the increased number of monitored ions in a given retention time window. To minimize such interferences and improve the instrument sensitivity a previously reported analytical method using GC-ECNI-LRMS combined with mathematical calculation was used.[1-4,7,8] Therefore, to eliminate interferences from congener groups with five carbon atoms more and two chlorine atoms less, all monitored ions of SCCPs and MCCPs were divided into four groups by mutual combination: C_{10}-C_{15}; C_{11}-C_{16}; C_{12}-C_{17}; and C_{13}-C_{14}. For each sample, four individual injections were performed. The congeners of SCCPs and MCCPs that could interfere with each other were categorized as one group, which not only reduce the numbers of monitored ions but also help to divide retention time windows. This method combined with the mathematical quantification deconvolution can effectively identify and eliminate the interferences of the simultaneous detection of SCCP and MCCP congener groups. SCCP and MCCP congener groups in a sample were distinguished by comparison of retention time, signal shape, and correct isotope ratio. If the interferences were found by identification, the peak signal of the monitored $[M\text{-}Cl]^-$ ion in SIM chromatogram is considered as common contributions of these congeners with same nominal mass from SCCP and MCCP congener groups.

Quantification equations of SCCPs and MCCPs.

The quantification of SCCPs and MCCPs were performed using the following equations 1-5:[3]

$$\text{Relative total CP area} = \sum_i \frac{\text{area } i\text{(congenre group)}}{\text{area } i \text{ (ISTD)}} \quad (1)$$

$$\text{Total response factor (CP mixture)} = \frac{\text{rel. total CP area (STD)}}{\text{amount CPs (STD)}} \quad (2)$$

$$\text{Chlorine content (CP mixture)} = \sum_i \frac{\text{rel. area (congener group } i\text{)}*\text{chlorine content (congener group } i\text{)}}{\text{rel.total CP area}} \quad (3)$$

$$\text{Total response factor (CPs in the sample)} = ax + b \quad (4)$$

$$\text{CP amount (sample)} = \frac{\text{relative total area (sample)}}{\text{total response factor (calculated for the sample)}} \quad (5)$$

Where "i" represents the CP congener group, ISTD the internal standard, STD the standard, "a" is the slope of the linear regression, "x" the chlorine content and "b" the axis intercept.

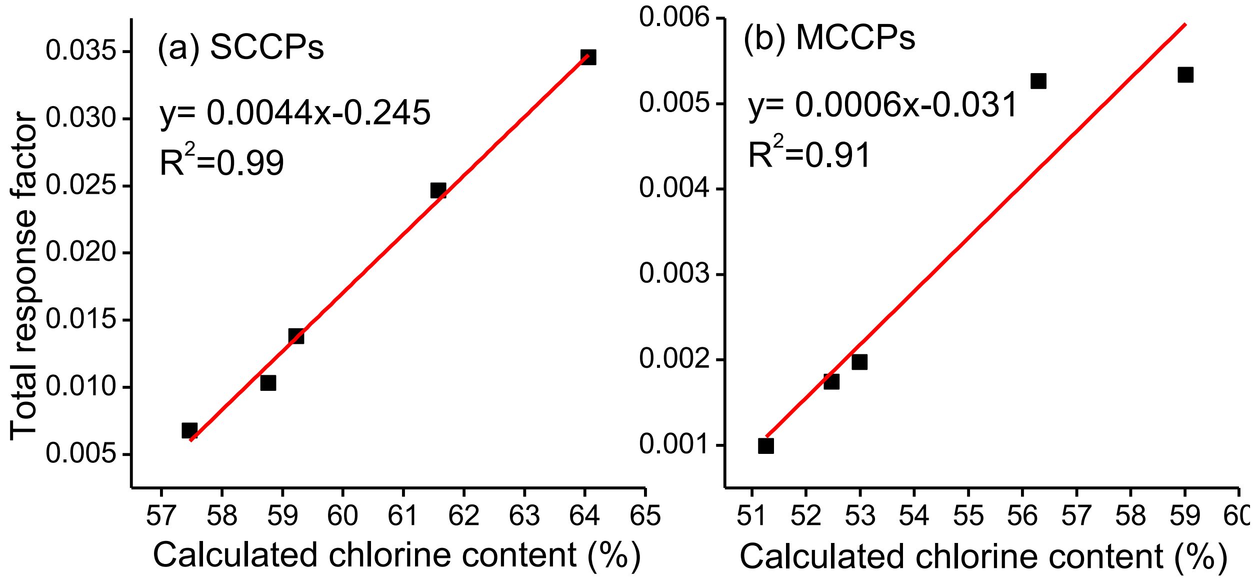

Figure S1. The calibration curves between the response factors of (a) SCCPs and (b) MCCPs and the calculated chlorine contents of the standard mixtures. To establish these calibration curves, five different SCCP standard mixtures with reported degrees of chlorination 51.5, 53.5, 55.5, 59.2, and 63 %Cl were measured, and the corresponding calculated chlorine contents were 57.5, 58.8, 59.2, 61.6, and 64 %Cl. Whereas for MCCPs, five standard mixtures with reported degrees of chlorination 42, 47, 52, 54.5, and 57 %Cl were measured, and the corresponding calculated chlorine contents were 51.3, 52.5, 53, 56.3, and 59 %Cl. The chlorination degrees on the x-axis represent the calculated chlorination degrees. SCCP and MCCP standards (100 ng/μL in cyclohexane) used for the establishment of linear function were obtained from Dr. Ehrenstorfer GmbH (Augsburg, Germany).

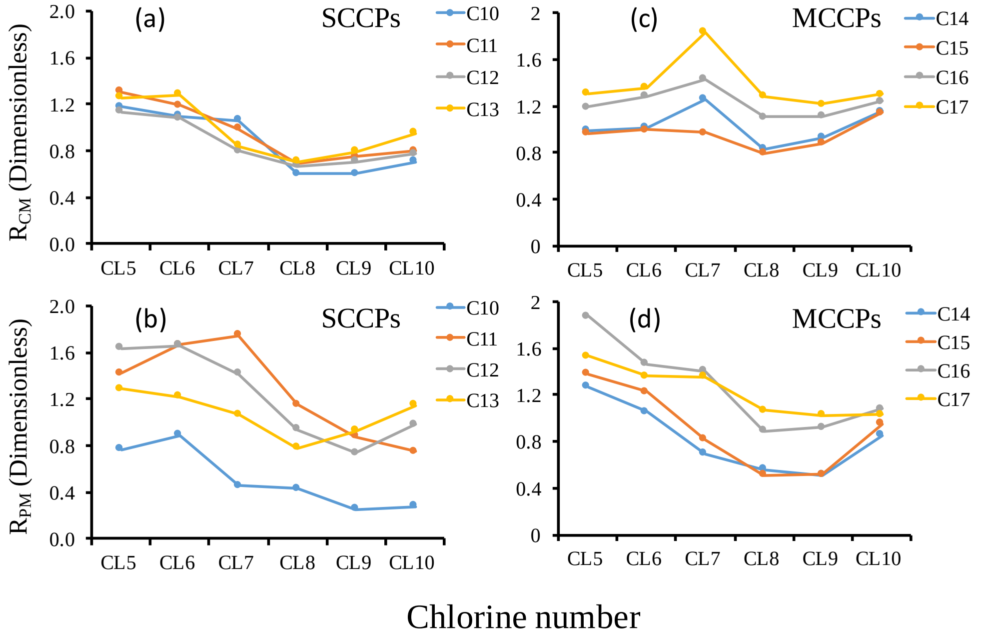

Figure S2. Chlorine atom-specific maternal to cord (R_{CM}) and maternal to placenta (R_{PM}) transfer efficiencies of [(a) and (b)] SCCPs and [(c) and (d)] MCCPs, respectively. The ratios are calculated based on average chlorine content.

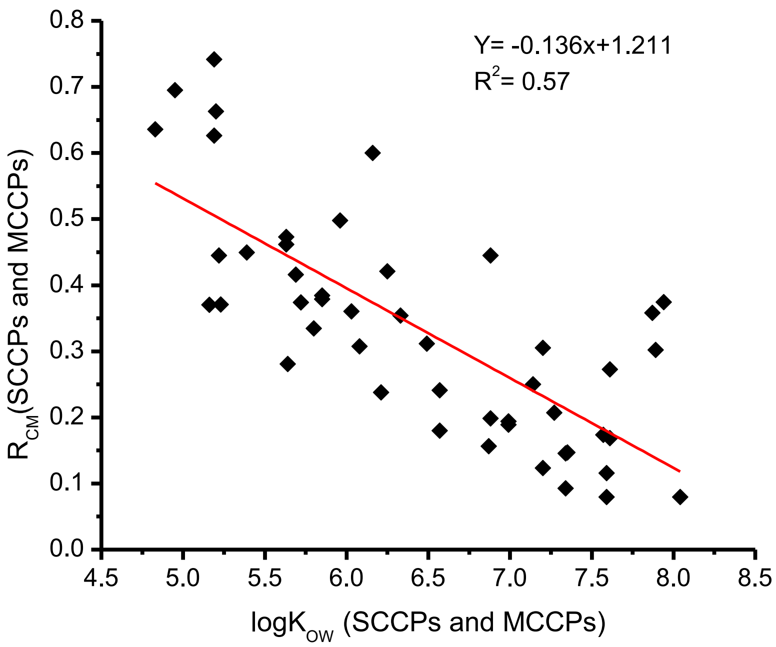

Figure S3. Relationship between the logK_{ow} and R_{CM} values of SCCPs and MCCPs.

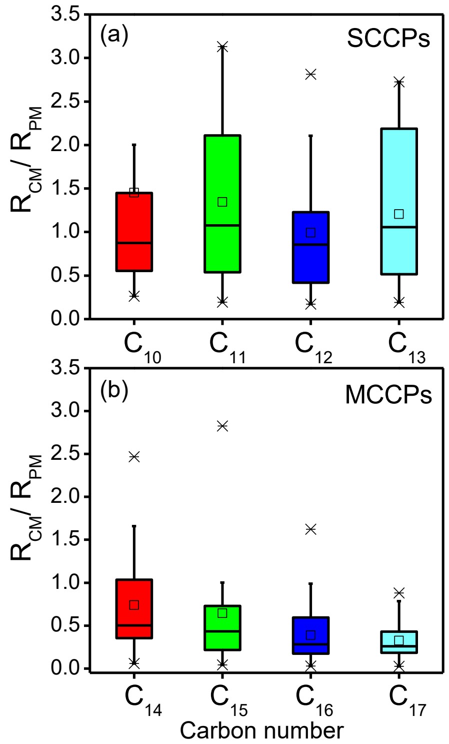

Figure S4. Placenta transfer efficiencies of (a) SCCP and (b) MCCP congener groups. The boxes mark the 25th and 75th percentiles. Small squares within the boxes indicate mean values. The bands inside the boxes indicate the median values. The whiskers represent 5th and 95th percentiles. The crosses above and below the whiskers indicate outlier values.

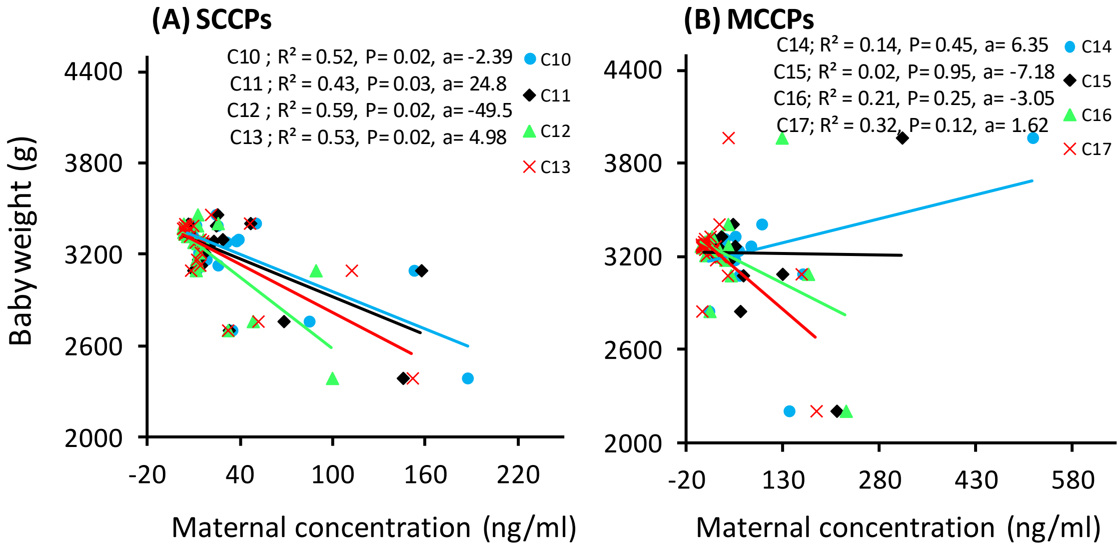

Figure S5. The relationship of maternal concentrations of (A) SCCPs and (B) MCCPs with baby body weight (g). In the legend, "R" and "a" represent the regression coefficient and regression slope, respectively.

Table S1. Detailed information of the degree of chlorination used to produce the calibration curves of standard mixtures of SCCPs and MCCPs.

Standards Solutions	S1	S2	S3	S4	S5
SCCPs					
51.5%	2	1	-	-	-
55.5%	-	1	2	1	-
63%	-	-	-	1	2
Degree of chlorination	51.5%	53.5%	55.5%	59.2%	63%
MCCPs					
42%	2	1			
52%	-	1	2	1	
57%	-	-		1	2
Degree of chlorination	42%	47%	52%	54.5%	57%

Note: Five standard mixtures of CPs with different degrees of chlorine were used to establish linear calibration curves. SCCPs with 53.5% chlorine content were obtained by mixing 51.5% and 55.5% of SCCPs at a ratio of 1:1 by volume. SCCPs with 59.2% chlorine content were obtained by mixing 55.5% and 63% of SCCPs at a ratio of 1:1 by volume. MCCPs with 47% degree of chlorination were obtained by mixing MCCPs of 42% and 52% at a volume ratio 1:1. MCCPs with 54.5% chlorine content were obtained by mixing 52% and 57% of MCCPs at a ratio of 1:1 by volume.

Table S2. Demographic characteristics of the mothers and neonates.

		Counts	Range	%/or Median
Mother Characteristics				
mother age (year)			21-33	27
pre-pregnancy body mass index (BMI) (kg m^{-3})			16.6-31.1	20.0
pregnancy weight gain (kg)			7-23	15
maternal serum albumin (g/L)			27.0-79.6	36.0
maternal serum total protein (g/L)			49.2-84.2	70.1
parity	primiparous	15		48.4
	multiparous	16		51.6
abortion	zero	16		51.6
	one	12		38.7
	two	1		3.2
	three	2		6.4
diet preference	vegetables	16		53.1
	meat	12		37.5
	seafood	3		9.4
drinking water source	tap water	25		81.2
	filtered tap water	6		18.8
alcohol drinking habit	nondrinker	30		96.9
	drinker	1		3.1
smoking habit	nonsmoker	29		93.7
	smoker	2		6.3
occupation	technician	3		9.7
	public servant	2		6.5
	business owner	5		16.1
	management	3		9.7
	industrial worker	2		6.5
	unemployed	8		25.8
	other	8		25.8
Neonate Characteristics				
gender	male	17		54.8
	female	14		45.2
body weight (g)			1990-4460	3313
head circumference (cm)			30-38	34
fetus gestational age (weeks)			36-45	38

Table S3. SCCP and MCCP congener groups and the two most abundant $[M\text{-}Cl]^-$ isotope fragment ions m/z values. The $[M\text{-}Cl]^-$ ions were monitored in the ECNI mode.

SCCPs	CL%	Monitored quantitative ions m/z values	Monitored qualitative ions m/z values	MCCPs	CL%	Monitored quantitative ions m/z	Monitored qualitative ions m/z
$C_{10}H_{17}Cl_5$	56.4%	279	277	$C_{14}H_{25}Cl_5$	47.8%	333	335
$C_{10}H_{16}Cl_6$	61.0%	313	315	$C_{14}H_{24}Cl_6$	52.5%	369	371
$C_{10}H_{15}Cl_7$	64.7%	347	349	$C_{14}H_{23}Cl_7$	56.5%	403	405
$C_{10}H_{14}Cl_8$	67.9%	381	383	$C_{14}H_{22}Cl_8$	59.8%	437	439
$C_{10}H_{13}Cl_9$	70.5%	415	417	$C_{14}H_{21}Cl_9$	62.8%	473	471
$C_{10}H_{12}Cl_{10}$	72.8%	449	451	$C_{14}H_{20}Cl_{10}$	65.3%	505	507
$C_{11}H_{19}Cl_5$	54.0%	293	291	$C_{15}H_{27}Cl_5$	46.1%	349	347
$C_{11}H_{18}Cl_6$	58.6%	327	329	$C_{15}H_{26}Cl_6$	50.8%	383	381
$C_{11}H_{17}Cl_7$	62.4%	361	363	$C_{15}H_{25}Cl_7$	54.7%	417	415
$C_{11}H_{16}Cl_8$	65.7%	395	397	$C_{15}H_{24}Cl_8$	58.1%	451	449
$C_{11}H_{15}Cl_9$	68.4%	429	431	$C_{15}H_{23}Cl_9$	61.1%	485	487
$C_{11}H_{14}Cl_{10}$	70.8%	463	465	$C_{15}H_{22}Cl_{10}$	63.7%	521	519
$C_{12}H_{21}Cl_5$	51.7%	307	305	$C_{16}H_{29}Cl_5$	44.5%	363	361
$C_{12}H_{20}Cl_6$	56.4%	341	343	$C_{16}H_{28}Cl_6$	49.1%	397	395
$C_{12}H_{19}Cl_7$	60.3%	375	377	$C_{16}H_{27}Cl_7$	53.1%	431	429
$C_{12}H_{18}Cl_8$	63.6%	409	411	$C_{16}H_{26}Cl_8$	56.5%	465	463
$C_{12}H_{17}Cl_9$	66.4%	443	445	$C_{16}H_{25}Cl_9$	59.5%	501	503
$C_{12}H_{16}Cl_{10}$	68.9%	479	477	$C_{16}H_{24}Cl_{10}$	62.1%	535	533
$C_{13}H_{23}Cl_5$	49.7%	321	323	$C_{17}H_{31}Cl_5$	43.0%	377	375
$C_{13}H_{22}Cl_6$	54.4%	355	357	$C_{17}H_{30}Cl_6$	47.6%	411	409
$C_{13}H_{21}Cl_7$	58.3%	389	391	$C_{17}H_{29}Cl_7$	51.5%	445	443
$C_{13}H_{20}Cl_8$	61.7%	423	425	$C_{17}H_{28}Cl_8$	55.0%	477	479
$C_{13}H_{19}Cl_9$	64.5%	459	457	$C_{17}H_{27}Cl_9$	58.0%	515	513
$C_{13}H_{18}Cl_{10}$	67.0%	493	491	$C_{17}H_{26}Cl_{10}$	60.6%	549	547

Table S4. Detection frequencies of SCCP and MCCP congener groups in all samples.

	SCCPs Detection Frequency (%)				**MCCPs Detection Frequency (%)**		
SCCPs	Maternal	Placenta	Cord	**MCCPs**	Maternal	Placenta	Cord
C10CL5	100	100	100	C14CL5	100	100	100
C10CL6	100	100	100	C14CL6	100	100	100
C10CL7	100	100	100	C14CL7	100	100	100
C10CL8	100	100	100	C14CL8	100	100	100
C10CL9	100	94	97	C14CL9	100	100	100
C10CL10	97	84	94	C14CL10	97	100	96
C11CL5	100	100	100	C15CL5	100	100	100
C11CL6	100	100	100	C15CL6	100	100	100
C11CL7	100	100	100	C15CL7	100	100	100
C11CL8	100	100	100	C15CL8	100	100	100
C11CL9	97	84	94	C15CL9	100	84	82
C11CL10	100	100	100	C15CL10	88	87	85
C12CL5	100	100	100	C16CL5	100	100	100
C12CL6	100	100	100	C16CL6	97	100	100
C12CL7	100	100	100	C16CL7	100	100	100
C12CL8	100	97	100	C16CL8	100	100	100
C12CL9	100	84	100	C16CL9	100	100	100
C12CL10	84	80	79	C16CL10	89	85	83
C13CL5	100	97	100	C17CL5	100	100	97
C13CL6	100	100	100	C17CL6	100	100	94
C13CL7	100	100	100	C17CL7	100	97	89
C13CL8	100	100	100	C17CL8	94	97	84
C13CL9	90	86	88	C17CL9	97	94	81
C13CL10	87	82	83	C17CL10	82	91	78

Table S5. Descriptive statistics of SCCP and MCCP congener groups in matched maternal serum, cord serum and placenta (samples n= 31, serum (ng/ml) and placenta (ng/g)).

	SCCP Concentrations				**MCCP Concentrations**		
	Range	**Mean**	**Median**		**Range**	**Mean**	**Median**
Maternal Serum							
Cl (%)	58.3-64.60	60.6	60.4	Cl (%)	50.2-57.9	52.9	52.8
C10	5.68-187.2	35.0	21.4	C14	13.9-518.3	89.8	39.9
C11	3.72-157.3	27.0	16.7	C15	7.37-315.1	59.1	34.0
C12	2.20-99.51	18.3	11.4	C16	2.14-227.8	37.6	18.5
C13	2.28-151.6	22.9	11.8	C17	3.19-181.7	28.7	13.7
Cl5	1.43-25.57	12.9	13.7	Cl5	1.16-20.44	10.8	10.7
Cl6	8.08-21.41	14.0	14.4	Cl6	6.79-16.61	12.9	13.4
Cl7	6.24-37.13	13.7	11.9	Cl7	6.34-23.54	14.6	13.8
CL8	2.61-18.90	9.46	8.49	Cl8	4.30-19.75	9.39	8.93
Cl9	2.03-17.34	6.80	5.71	Cl9	1.79-7.440	3.71	3.36
Cl10	1.05-8.910	3.82	3.14	Cl10	0.47-3.240	1.57	1.47
∑SCCP	15.9-583.7	103	66.2	∑MCCP	29.33-1006	215	126
Cord Serum							
Cl (%)	58.4-62.6	59.6	59.4	Cl (%)	50.7-54.9	53.2	53.2
C10	3.33-111.2	18.7	12.5	C14	6.01-43.75	20.2	16.1
C11	1.73-70.09	15.4	10.8	C15	2.86-34.99	12.8	8.53
C12	0.99-19.21	6.58	5.59	C16	1.15-11.49	5.27	4.76
C13	0.94-39.30	9.27	6.80	C17	1.21-5.30	3.22	3.07
Cl5	3.34-22.70	16.1	16.4	Cl5	5.77-20.63	10.6	10.5
Cl6	9.77-24.1	16.2	16.1	Cl6	8.47-14.30	11.2	10.8
Cl7	6.13-33.29	13.4	11.1	Cl7	11.9-20.30	15.4	15.3
Cl8	2.24-15.19	6.25	5.82	Cl8	4.99-14.45	8.44	8.16
Cl9	1.54-11.11	4.67	4.40	Cl9	2.28-6.280	4.09	3.94
Cl10	1.21-5.75	2.96	2.75	Cl10	1.31-6.67	3.46	3.31
∑SCCP	8.46-222.6	49.9	36.7	∑MCCP	13.60-90.12	41.5	34.2
Placenta							
Cl (%)	58.3-61.2	58.9	58.8	Cl (%)	50.1-54.1	51.8	51.6
C10	3.56-33.36	14.4	12.4	C14	12.9-211.4	41.0	21.9
C11	2.53-35.22	11.8	09.4	C15	7.11-159.9	33.6	20.9
C12	1.77-36.55	7.63	4.88	C16	1.64-159.0	25.5	16.4
C13	1.95-40.72	8.59	6.45	C17	3.22-112.0	17.8	9.73
Cl5	3.53-22.47	15.3	15.8	Cl5	7.63-20.67	15.5	15.2
Cl6	10.3-24.12	17.7	16.8	Cl6	8.13-13.96	11.3	11.2
Cl7	8.76-19.78	12.4	12.1	Cl7	6.66-17.95	12.5	12.8
Cl8	4.16-15.51	7.17	7.06	Cl8	4.42-12.29	5.89	5.55
Cl9	2.27-8.170	3.97	3.64	Cl9	2.02-17.96	4.73	2.90
Cl10	1.21-3.970	2.38	2.20	Cl10	1.16-3.99	1.85	1.68
∑SCCP	10.2-131.7	42.4	33.1	∑MCCP	24.8-642.3	118	68.3

Table S6. Analysis of variance test (ANOVA) for comparisons of SCCP and MCCP concentrations in maternal sera, cord sera, and placenta.

Sample	(I) CPs	(J) CPs	Mean Difference (I-J)	Std. Error	Sig.*	95% Confidence Interval for Difference Lower Bound	95% Confidence Interval for Difference Upper Bound
Maternal	SCCPs	MCCPs	-115.679*	32.737	.001	-180.276	-51.082
Placenta	SCCPs	MCCPs	-77.102*	32.737	.020	-141.699	-12.505
Cord	SCCPs	MCCPs	9.261	32.737	.778	-55.336	73.858
CPs	**(I) sample**	**(J) sample**	**Mean Difference (I-J)**	**Std. Error**	**Sig. ***	**95% Confidence Interval for Difference Lower Bound**	**95% Confidence Interval for Difference Upper Bound**
SCCPs	Maternal	Placenta	55.943	32.737	.089	-8.654	120.540
	Placenta	Cord	-8.389	32.737	.798	-72.986	56.208
	Cord	Maternal	-47.553	32.737	.148	-112.150	17.044
MCCPs	Maternal	Placenta	94.520*	32.737	.004	29.923	159.117
	Placenta	Cord	77.975*	32.737	.018	13.378	142.571
	Cord	Maternal	-172.494*	32.737	.000	-237.091	-107.897

*. The mean difference is significant at the 0.05 level.

Table S7. The log K_{OW} values of SCCPs and MCCPs, derived from Glüge et al.[9]

SCCPs	log K_{OW}	MCCPs	log K_{OW}
$C_{10}H_{17}Cl_5$	4.83	$C_{14}H_{25}Cl_5$	6.88
$C_{10}H_{16}Cl_6$	4.95	$C_{14}H_{24}Cl_6$	6.57
$C_{10}H_{15}Cl_7$	5.19	$C_{14}H_{23}Cl_7$	6.57
$C_{10}H_{14}Cl_8$	5.16	$C_{14}H_{22}Cl_8$	6.87
$C_{10}H_{13}Cl_9$	5.39	$C_{14}H_{21}Cl_9$	6.21
$C_{10}H_{12}Cl_{10}$	5.63	$C_{14}H_{20}Cl_{10}$	7.2
$C_{11}H_{19}Cl_5$	5.19	$C_{15}H_{27}Cl_5$	7.14
$C_{11}H_{18}Cl_6$	5.2	$C_{15}H_{26}Cl_6$	6.99
$C_{11}H_{17}Cl_7$	5.22	$C_{15}H_{25}Cl_7$	6.99
$C_{11}H_{16}Cl_8$	5.23	$C_{15}H_{24}Cl_8$	6.88
$C_{11}H_{15}Cl_9$	5.63	$C_{15}H_{23}Cl_9$	7.61
$C_{11}H_{14}Cl_{10}$	5.96	$C_{15}H_{22}Cl_{10}$	7.94
$C_{12}H_{21}Cl_5$	5.85	$C_{16}H_{29}Cl_5$	7.61
$C_{12}H_{20}Cl_6$	5.69	$C_{16}H_{28}Cl_6$	7.34
$C_{12}H_{19}Cl_7$	5.8	$C_{16}H_{27}Cl_7$	7.34
$C_{12}H_{18}Cl_8$	5.64	$C_{16}H_{26}Cl_8$	7.2
$C_{12}H_{17}Cl_9$	5.72	$C_{16}H_{25}Cl_9$	7.27
$C_{12}H_{16}Cl_{10}$	6.03	$C_{16}H_{24}Cl_{10}$	7.89
$C_{13}H_{23}Cl_5$	6.25	$C_{17}H_{31}Cl_5$	8.04
$C_{13}H_{22}Cl_6$	6.16	$C_{17}H_{30}Cl_6$	7.59
$C_{13}H_{21}Cl_7$	6.08	$C_{17}H_{29}Cl_7$	7.59
$C_{13}H_{20}Cl_8$	6.49	$C_{17}H_{28}Cl_8$	7.35
$C_{13}H_{19}Cl_9$	5.85	$C_{17}H_{27}Cl_9$	7.57
$C_{13}H_{18}Cl_{10}$	6.33	$C_{17}H_{26}Cl_{10}$	7.87

Maternal-Cord	Levene's Test for Equality of Variances		t-test for Equality of Means						
					Sig. *	Mean	Std. Error	95% Confidence Interval	
SCCPs	F	Sig.	t	df	(2-tailed)	Difference	Difference	Lower	Upper
C10-C10	5.503	.022	1.870	42.46	.066	16.32337	8.72944	-1.28774	33.93448
C11-C11	3.853	.054	1.641	40.74	.106	11.56832	7.05121	-2.67469	25.81134
C12-C12	12.52	.001	2.789	32.46	.007	11.73283	4.20717	3.16787	20.29780
C13-C113	9.762	.003	2.284	33.67	.026	13.64090	5.97234	1.49925	25.78256
MCCPs									
C14-C14	20.043	.000	3.197	30.61	.002	69.59255	21.76500	25.17980	114.00530
C15-C15	17.775	.000	3.733	31.27	.000	46.33829	12.41395	21.02887	71.64771
C16-C16	21.309	.000	3.501	30.13	.001	32.33748	9.23673	13.47707	51.19789
C17-C17	19.244	.000	3.349	30.05	.002	25.48384	7.60938	9.94448	41.02320

Table S8. Independent samples T-test between the CP congener groups of maternal sera and cord sera.

*. The difference is significant at the 0.05 level.

Table S9. Independent samples T-test between the R_{CM}/R_{PM} Ratios of SCCP and MCCP congener groups.

Ratios	Levene's Test for Equality of Variances		t-test for Equality of Means						
								95% Confidence Interval of the Difference	
	F	Sig.	t	df	Sig. * (2-tailed)	Mean Difference	Std. Error Difference	Lower	Upper
SCCPs R_{CM}/R_{PM}									
C10-C11	.982	.326	-.741	56.700	.461	-.33498	.45180	-1.23980	.56983
C10-C12	1.939	.169	.906	47.954	.368	.29116	.32120	-.35467	.93698
C10-C13	.288	.594	-.285	59.960	.777	-.11059	.38853	-.88778	.66659
C11-C12	5.512	.022	1.604	41.703	.114	.62614	.39040	-.16189	1.41417
C11-C13	.355	.554	.501	56.047	.618	.22439	.44744	-.67192	1.12070
C12-C13	5.567	.022	-1.275	48.707	.207	-.40175	.31503	-1.03493	.23143
MCCPs R_{CM}/R_{PM}									
C14-C15	.003	.958	.625	60.773	.534	.09660	.15459	-.21254	.40574
C14-C16	7.842	.007	2.986	48.859	.004	.34691	.11619	.11340	.58041
C14-C17	15.762	.000	3.752	40.517	.000	.40863	.10892	.18859	.62867
C15-C16	5.185	.026	1.926	44.970	.039	.25031	.12998	-.01150	.51212
C15-C17	9.671	.003	2.526	38.225	.014	.31203	.12353	.06201	.56205
C16-C17	1.903	.173	.885	55.687	.379	.06172	.06973	-.07797	.20142

*. The difference is significant at the 0.05 level.

Table S10. Independent samples T-test for the R_{CM} and R_{PM} ratios between the lower and highly chlorinated congener groups of SCCPs and MCCPs.

	Levene's Test for Equality of Variances		t-test for Equality of Means						
								95% Confidence Interval of the Difference	
	F	Sig.	t	df	Sig. (2-tailed)	Mean Difference	Std. Error Difference	Lower	Upper
SCCPs									
R_{CM}									
Cl5-CLl0	10.027	.002	2.343	34.964	.022	1.26204	.53862	.18535	2.33874
Cl6-Cl9	4.591	.036	1.993	51.178	.041	.29279	.14691	-.00088	.58646
Cl7-Cl8	.002	.964	1.608	61.996	.113	.24428	.15187	-.05930	.54786
R_{PM}									
Cl5-Cl10	18.166	.000	3.059	33.582	.003	1.31214	.42888	.45481	2.16946
Cl6-Cl9	.252	.618	3.792	61.953	.000	.57729	.15225	.27296	.88163
Cl7-Cl8	4.033	.049	.033	46.146	.974	.00501	.15393	-.30270	.31272
MCCPs									
R_{CM}									
Cl5-Cl10	2.581	.113	-2.851	59.394	.006	-1.26845	.44490	-2.15838	-.37853
Cl6-Cl9	8.451	.005	-2.849	47.655	.006	-.33439	.11737	-.56917	-.09962
Cl7-Cl8	.664	.418	1.056	59.674	.295	.11532	.10919	-.10310	.33373
R_{PM}									
Cl5-Cl10	2.003	.162	1.333	45.940	.188	.60100	.45088	-.30089	1.50289
Cl6-Cl9	19.718	.000	-2.362	32.696	.021	-.37014	.15673	-.68366	-.05663
Cl7-Cl8	.732	.395	2.035	53.520	.040	.19101	.09384	.00330	.37872

*. The difference is significant at the 0.05 level.

Table S11. Linear regression equations between logC-logM[a] and logP-logM[a] for SCCP and MCCP congener groups.

Compound	Equation (C-M)	R, *P* values	Equation (P-M)	R, *P* values
SCCPs				
C10	logC = 0.6745M + 0.2155	R= 0.509, *P*= 0.003	logP = 0.3146M + 0.6744	R= 0.773, *P* = 0.000003
C11	logC = 0.5165 M + 0.4023	R= 0.462, *P*= 0.009	logP = 0.3524 M + 0.5405	R= 0.571, *P* = 0.001
C12	logC = 0.3964 M + 0.2966	R= 0.538, *P* = 0.002	logP = 0.3986 M + 0.3471	R= 0.528, *P* = 0.002
C13	logC = 0.4455 M + 0.3276	R= 0.522, *P* = 0.003	logP = 0.3909 M + 0.3692	R= 0.533, *P* = 0.002
MCCPs				
C14	logC = 0.2869 M + 0.7343	R= 0.451, *P* = 0.011	logP = 0.4252 M + 0.7475	R= 0.606, *P* = 0.0003
C15	logC = 0.0387 M + 0.9283	R= 0.049, *P* = 0.794	logP = 0.5473 M + 0.5091	R= 0.650, *P* = 0.0001
C16	logC = 0.0974 M + 0.5489	R= 0.219, *P* = 0.236	logP = 0.635 M + 0.388	R= 0.756, *P* = 0.000001
C17	logC = 0.074 M + 0.389	R= 0.200, *P* = 0.282	logP = 0.5369 M + 0.4472	R= 0.733, *P* = 0.000003

[a] M: maternal concentration; C: Cord concentration; P: Placenta concentration

** Correlation is significant at the 0.01 level (2-tailed).

* Correlation is significant at the 0.05 level (2-tailed).

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